Note on nonsymmetric finite differences for Maxwell's equations

Tobin A. Driscoll[1] and Bengt Fornberg[2]

Department of Applied Mathematics, CB526, University of Colorado, Boulder, CO 80309

E-mail: tad@colorado.edu, fornberg@colorado.edu

1. INTRODUCTION

It is well known that Maxwell's equations for a constant medium can be written in either a first-order or a second-order form. For the simple case of one space dimension and appropriate units, we have either

$$\begin{aligned} \frac{\partial E}{\partial t} &= \frac{\partial H}{\partial x}, \\ \frac{\partial H}{\partial t} &= \frac{\partial E}{\partial x}, \end{aligned} \tag{1}$$

or

$$\begin{aligned} \frac{\partial^2 E}{\partial t^2} &= \frac{\partial^2 E}{\partial x^2}, \\ \frac{\partial^2 H}{\partial t^2} &= \frac{\partial^2 H}{\partial x^2}. \end{aligned} \tag{2}$$

Numerical solution methods for discretizing second derivatives are available (for example, centered finite differences in space and Nyström or Störmer methods in time). These methods may have advantages in accuracy and stability over their first-derivative counterparts. However, the imposition of boundary conditions is more difficult in the second-order formulation.

Liu [2] proposed finite difference (FD) discretizations of the first-order form that target the second-order derivatives for accuracy. For example, we can discretize (1) in space by

$$\begin{aligned} \frac{\partial E_n}{\partial t} &= \frac{1}{h}(H_{n+1} - H_n), \\ \frac{\partial H_n}{\partial t} &= \frac{1}{h}(E_n - E_{n-1}). \end{aligned} \tag{3}$$

Note the different approximations used on the right-hand sides; they are both first-order accurate approximations of the derivatives in (1). However, one finds that

$$
\begin{aligned}
\frac{\partial^2 E_n}{\partial t^2} &= \frac{1}{h^2}(E_{n+1} - 2E_n + E_{n-1}), \\
\frac{\partial^2 H_n}{\partial t^2} &= \frac{1}{h^2}(H_{n+1} - 2H_n + H_{n-1}),
\end{aligned}
\tag{4}
$$

which are second-order accurate approximations of (2). Liu also proposed methods which were first-order accurate on (1) and as much as sixth-order accurate on (2) (we denote the accuracy of such a method by the pair (1,6)). In each case the coefficients in the discretization for H are the antisymmetric counterpart to those for E. The coefficients for each individual component do not themselves possess the usual antisymmetry seen in accurate FD for the first derivative, and for this reason they were called "nonsymmetric" in [2]. It is straightforward to find methods of this type with orders of accuracy $(p,2m-p-1)$ using m unknown coefficients.

In [2] numerical experiments seemed to confirm the relevance of the second-derivative accuracy. In each experiment a pulse was propagated in a periodic domain until such time as it had returned to its original position. In this note we show that such times—more precisely, integer multiples of half of the period—are special, and at all other times the accuracy is governed by the (relatively inaccurate) approximation to first derivative. In a nonperiodic problem these special times would not exist. We also show that the nonsymmetric methods are inaccurate at all times in the presence of variable coefficients. We present the results of a few experiments to verify our claims.

For the rest of this note we reserve the word "order" for reference to the order of accuracy of a method and use the terms "first-derivative" and "second-derivative" to describe the different PDE formulations.

2.   ANALYSIS

The general solution for each component of (2) is given by d'Alembert's formula. For example,

$$
E(x,t) = f(x - t) + f(x + t) + \int_{x-t}^{x+t} g(\xi)\, d\xi,
\tag{5}
$$

where

$$
\begin{aligned}
f(\xi) &= E(\xi, 0), \\
g(\xi) &= \frac{\partial E}{\partial t}(\xi, 0),
\end{aligned}
$$

with periodic extensions outside the original interval $x \in [-L, L]$. By the first-order formulation (1), $g(\xi) = \frac{\partial H}{\partial x}(\xi, 0)$.

The nonsymmetric FD methods are designed to be accurate representations of (2). However, $g(\xi)$ in d'Alembert's formula is replaced by

$$
\frac{\partial H}{\partial x}(\xi, 0) + h^p r(\xi),
\tag{6}
$$

where p is the order of accuracy of the FD method for the *first* derivative. Hence the same order of error remains in $E(x, t)$.

Note that the leading term in $r(\xi)$ is a higher-order derivative of $H(x,0)$. Thus r has no constant Fourier component. At the times $t = mL$, $m \in \mathbf{N}$, the integral in (5) is over m full periods of g, so the contribution of the error term in (6) vanishes. At those times, and only those times, the error is controlled by the accuracy of the second-derivative approximation to (2).

The nonsymmetric methods also run into trouble with variable coefficients. In the equations

$$\begin{aligned}
\frac{\partial E}{\partial t} &= \alpha(x)\frac{\partial H}{\partial x}, \\
\frac{\partial H}{\partial t} &= \beta(x)\frac{\partial E}{\partial x},
\end{aligned} \tag{7}$$

the correct second-derivative form for E is

$$\frac{\partial^2 E}{\partial t^2} = \alpha\beta\frac{\partial^2 E}{\partial x^2} + \alpha\beta'\frac{\partial E}{\partial x}.$$

But applying the method of (3) we get

$$\begin{aligned}
\frac{\partial^2 E_n}{\partial t^2} &= h^{-1}\alpha_n\left(\frac{\partial H_{n+1}}{\partial t} - \frac{\partial H_n}{\partial t}\right) \\
&= h^{-2}\alpha_n(\beta_{n+1}E_{n+1} - (\beta_{n+1} + \beta_n)E_n + \beta_{n-1}E_{n-1}) \\
&= \alpha_n(\beta_n\frac{\partial^2 E_n}{\partial x^2} + \beta'_n\frac{\partial E_n}{\partial x}) + \frac{1}{2}h\alpha_n(\beta''_n\frac{\partial E_n}{\partial x} + \beta'_n\frac{\partial^2 E_n}{\partial x^2}) + O(h^2),
\end{aligned}$$

and the method is only first-order accurate.

3. NUMERICAL EXPERIMENTS

In this section we validate the claims made above. We run the 1D Maxwell equations (1) on the periodic interval $x \in [-1, 1)$, with initial values

$$\begin{aligned}
E(x,0) &= e^{-30x^2}, \\
H(x,0) &= -e^{-30x^2}.
\end{aligned}$$

Although not naturally periodic, these functions are comparable to double precision round-off at the ends of the interval. In space we use the method called NS3 in [2], which is first order on the first derivative and 6th order on the second derivative. We time step using fourth-order Runge–Kutta with a time step $1/2048$, small enough so that all observed errors are due to spatial discretization only.

Figure 1 shows the error for 64 and 128 points at evenly spaced times from 0 to 2 (i.e., up to one full traversal). The vertical scale on the time series is $[-0.2, 0.2]$, indicating that the errors are quite large. Furthermore, the grid refinement reduces error by about half, consistent with first order accuracy. At the special times $t = 1$ and $t = 2$ the error is much smaller. The maximum errors at $t = 2$ are about 8.99×10^{-5} and 1.52×10^{-6}. Their ratio of about 60 implies an effective convergence order of 5.9.

We also tested the variable coefficient problem (7) with $\alpha(x) = 1 + 0.2\sin(\pi x)$, $\beta(x) = 1 - 0.2\cos(\pi x)$. The results are shown at the final time $t = 2$ in Fig. 2. The NS method of type (1,6) is now first order accurate even at the final time, while Yee's method [3] retains
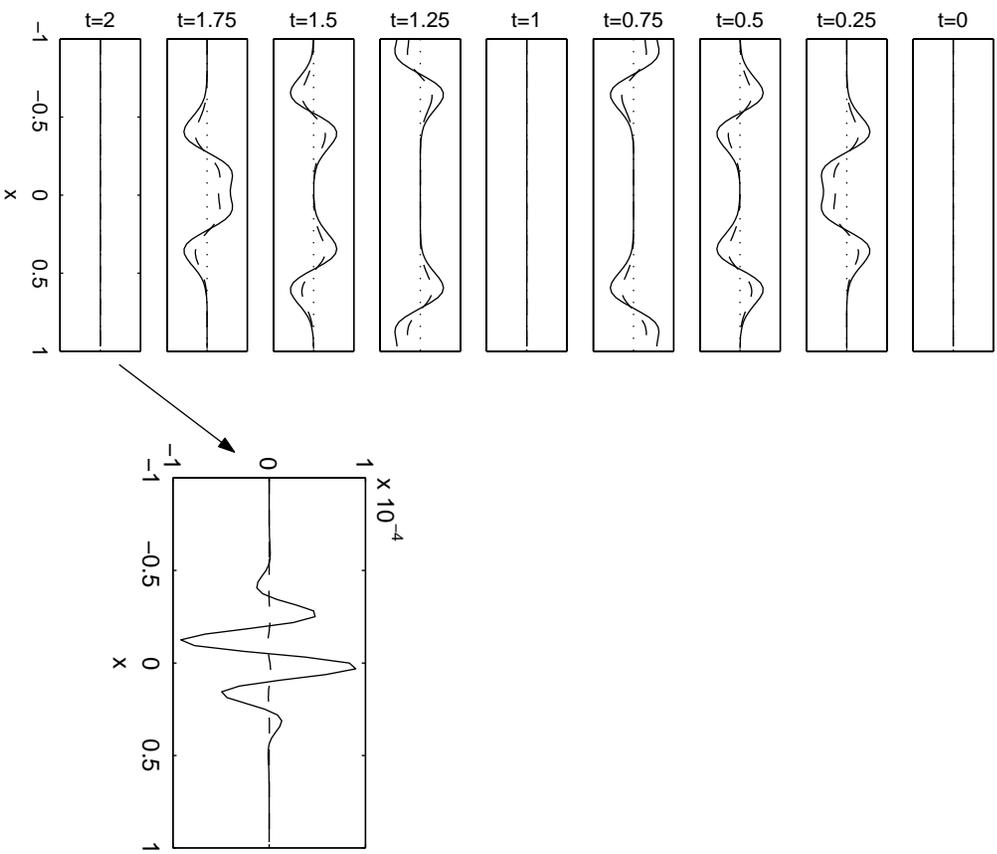
FIG. 1. Errors for an nonsymmetric FD method for periodic Maxwell's equations in 1D. Each curve is the difference between the numerical solution with 64 (solid) and 128 (dashed) points in $[-1, 1]$. The scale of each graph on the left is $[-0.2, 0.2]$, and a dotted line marks the zero level. The plot on the right is rescaled to better show the error at the final time.
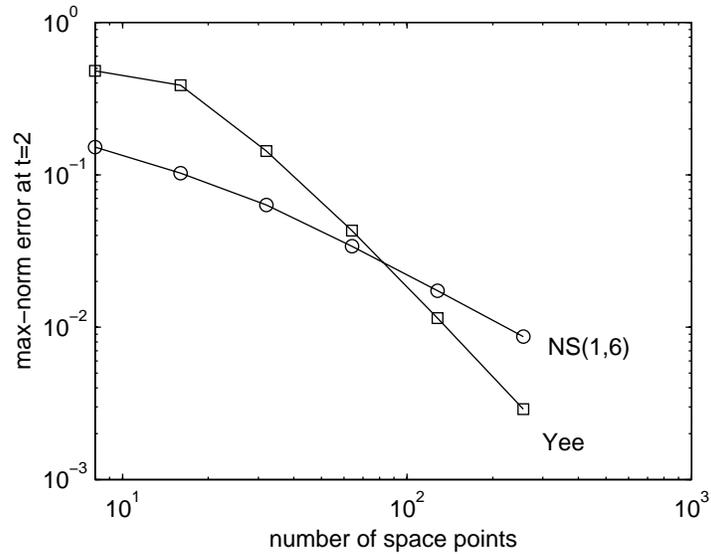
FIG. 2. Comparison of spatial discretizations for the variable-coefficient model problem (7) with slowly varying α and β. Here the "exact" solution is obtained from an 8th-order method at the finest discretization. The NS method is governed by the first-derivative accuracy, while standard methods such as Yee's are unaffected.

second-order accuracy. Any standard staggered or nonstaggered FD method [1] would be similarly unaffected.

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